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A DOCKING MOLECULAL CALCULATIONS TO STUDY THE PROPERTIES OF THE D-MANNOSE AS A NATURAL TREATMENT OF URINARY INFECTIONS CAUSED BY E. COLI

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D-mannose is a natural sugar present in various foods, and binds to *E. coli,* which is then discharged through urine. The purpose of this research is to prove the efficiency of D-mannose and provide an approach to the mean duration of treatment by performing tests on laboratory rats, by provocation of urinary tract infection (UTI). This was done by infecting the rats by different ways and then administration of D-mannose orally. A bacteriological examination of urine was carried out and the interpretation of results was based on the sterility of the culture media. Another aim of this research is the study of protein-protein interactions, which have an important role to understand the process of pathogenesis of bacterial and viral infections. Bioinformatics analysis contributes to the study of protein-protein interactions with the help of softwares for molecular dynamics and protein-protein docking. We have studied the interaction between D-mannose and the FimH protein by using molecular dynamics. Initially, several structural calculations and optimizations by Hyperchem8 software were conducted on D-mannose to understand how the natural sugar attacks the *E. coli* bacterium. Then docking calculations were performed by Hex6.3. Interpretation of results is based on the energy of interaction formed by ligands α-D-mannose and β-D-mannose. The lowest energy of interaction of complex probably presents a greater inhibition of FimH protein.

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